VNIVERSITAT DE VALÈNCIA

Course Guide
34062 Organic Chemistry

COURSE DATA

Data Subject	
Code	34062
Name	Organic Chemistry
Cycle	Grade
ECTS Credits	12.0
Academic year	2017 - 2018

Study (s)

Degree	Center	Acad. year	Period
1201 - Degree in Pharmacy	Faculty of Pharmacy and Food Sciences	2	Annual
1211 - D.D. in Pharmacy-Human Nutrition and Dietetics	Faculty of Pharmacy and Food Sciences	2	Annual

Subject-matter

Degree	Subject-matter	Character
1201 - Degree in Pharmacy	2 - Organic chemistry	Obligatory
1211 - D.D. in Pharmacy-Human Nutrition and Dietetics	1 - Asignaturas obligatorias del PDG Farmacia-Nutrición Humana y Dietética	Obligatory

Coordination

Name	Department
BALLESTEROS CAMPOS, RAFAEL	325 - Organic Chemistry

SUMMARY

Knowledge of the structure and reactivity of organic compounds is essential for a good understanding of the biochemical processes, metabolism and toxicology of drugs, and their mechanism of action at the molecular level. Moreover, this knowledge is also necessary to raise the preparation of compounds that retain all their beneficial properties but not have unwanted side effects.

The course has been organized into two semesters, the first with more theoretical content than the second one. In the first half , the contents of the theoretical part of this subject have been structured around the study of the most important and frequent functional groups in organic compounds. Since students have taken chemistry courses in the first year, it will be necessary simply remember and reinforce basic concepts about the structure and types of bonds in these compounds, which students should know,

showing particular attention to the intermolecular forces, so important in the processes of enzyme-substrate or drug-receptor recognition. Also we consider necessary to show how to apply to organic compounds the existing knowledge about acidity and basicity, as well as thermodynamics and kinetics in chemical reactions.

In the second half, the contents of the theoretical work will focus on basic aspects of synthetic transformations of organic compounds, and also on the application of spectroscopic techniques in the structural elucidation. At the same time, in the practical sessions conducted in the laboratory, students will start in the use of standard techniques of manipulation, isolation, identification and transformation of organic compounds.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Basic knowledge of general chemistry both at theoretical (atomic structure and chemical bonding, kinetics and thermodynamics applied to chemical processes, acidity and basicity, ..) and practical (correct use of the material commonly used in a chemistry lab, simple operations of separation, preparation of solutions, implementing the appropriate safety standards) levels.

OUTCOMES

1201 - Degree in Pharmacy

- To know how interpret, value and communicate relevant data in the different aspects of pharmaceutical activity, making use of information and communication technologies.
- Skill to communicate ideas, analyze problems and solve them with a critical mind, achieving team-working abilities and assuming leadership whenever required.
- Develop know-hows for their professional career.
- Ability to seek and find knowledge related to the area, always applying the critical and self-critical capacity.
- Module: Chemistry - To know and apply the main structural research techniques including spectroscopy.
- To recognize the bond types that can be present in organic compounds.
- To understand and know how to use the different representations of organic molecules.
- To know how to apply the general rules of nomenclature of organic compounds, including stereochemistry.

- To identify the different functional groups present in organic molecules and to know how to relate their presence with the physicochemical properties of organic molecules.
- To know the general reactivity of the most important functional groups present in organic molecules.
- To know the mechanisms of the most important chemical transformations.
- To know the more general methods to obtain the different types of compounds.
- To know how to relate the presence of functional groups in the molecules with their reactivity in different reaction types (substitutions, eliminations, additions, etc.)
- To understand and to be able to predict the behaviour of organic compounds in different environments (chemical, biological, environmental)
- To be able to design synthesis of simple organic compounds from certain starting reagents and involving more than one reaction.
- To know how to apply the basic techniques of synthesis, isolation and characterization for organic compounds.
- To know the risks associated to the use of organic compounds and the techniques used in their handling, preparation, isolation, purification and analysis.

LEARNING OUTCOMES

In this course students will acquire the following skills and abilities:
* Representing organic molecules through the most common methods of representation.
* Recognizing the stereochemistry of organic compounds.
* Identifying the organic functional groups and apply the rules of nomenclature.
* Identifying the possible intermolecular forces between the different compounds depending on the structure of functional groups they contain.
* Predicting the acid-base behavior of organic molecules
* Knowing the characteristic reactivity of each functional group.
* Understanding the most important methods for the preparation of the different functional groups.
* Understanding and learning to use the reaction mechanisms as logical interpretations of the reactions studied.
* Designing simple synthesis.
* Relating the knowledge acquired during the course with the reactions that take place in metabolic processes.
* Knowing and using the most common techniques used in the separation, identification and preparation of simple organic compounds.

DESCRIPTION OF CONTENTS

1. Basic concepts: Structure, reaction mechanisms.

Part I: 10h.

STRUCTURE AND BONDING IN ORGANIC COMPOUNDS.- Introduction .- Functional Groups .- Structural formula and systematic nomenclature .- Lewis Formula.- Molecular Geometry .Covalent bond in carbon compounds. Polarity in organic molecules.- Aromaticity:- Intermolecular Forces.- Molecular models.

REACTION MECHANISMS.- Types of organic reactions .- Thermodynamics and kinetics.- Profiles and reaction mechanisms .- Polar reactions: nucleophile and electrophile.- Radical reactions Reaction intermediates: radicals, carbanions, carbocations and carbenes.

ACID-BASE REACTION IN ORGANIC COMPOUNDS.- Structural and electronic factors influencing the acidity and basicity: inductive effect, conjugation and aromaticity. Polyfunctional acids and bases.- Amphoteric compounds .- Aminoacids.- Influence of pKa in the absorption of drugs.

2. Hydrocarbons;Stereochemistry.

Part II: - 10 h.

ALKANES AND CYCLOALKANES .- Structure.- Physical Properties .- Conformational analysis of ethane and butane .- Cycloalkanes .- Ring Strain.- Cyclohexane.- Substituted cyclohexanes: cis-trans isomerism.- Bigger cycloalkanes and polycyclic alkanes.- Steroids.- REACTIVITY: Combustion.- Halogenation of alkanes: mechanism.-Relative stability of radicals.

STEREOCHEMISTRY Stereoisomers .- Conformational and configurational isomers.- Stereogenic centers.- Optical and geometric isomers .- Convention E-Z in alkenes.- Chirality:- Optical activity.- Racemates .- The rule RS : Nomenclature of enantiomers: .- Fischer projections .-D and L Configurations - Compounds containing more than one stereocenter.- Diastereomers .- Meso compounds.- Resolution of a racemic mixture.

ALKENES, ALKYNES AND CONJUGATED SYSTEMS .- Physical properties of alkenes.- Relative stabilities of alkenes. -Reactivity: Polar addition of symmetrical and unsymmetrical electrophiles.- Stability of carbocations .- Regioselectivity - Catalytic hydrogenation.- Oxidation .- Reactions of alkynes.- Acidity of terminal alkynes .- Electrophilic addition in conjugated systems.

AROMATIC COMPOUNDS.- Benzene.- Nomenclature of substituted benzenes.- Aromatic and heteroaromatic rings.- Electrophilic aromatic substitution. Halogenation, nitration and sulfonation .- Friedel-Crafts reaction .- Activation and deactivation of the benzene ring .- Orientation in electrophilic aromatic substitution.- Nucleophilic aromatic substitution. -Polycyclic aromatic hydrocarbons.- Reactivity of the benzyl system.

3. Compounds with simple carbon-heteroatom bond

Part III: 12h

HALOGENATED ORGANIC COMPOUNDS .- Structure and physical properties of haloalkanes .- Nucleophilic Substitution.- Synthetic applications .- SN1 and SN2 mechanisms.- Dehydrohalogenation: Elimination Reaction Mechanisms .- E1 and E2 mechanisms.- Competition between substitution and elimination. - Some applications of halogenated derivatives.- Organometallic reagents: Structure and reactivity.

ALCOHOLS, PHENOLS AND THIOLS .- Structure and physical properties of alcohols .- Nomenclature of alcohols and phenols Acidity and basicity .- Preparation of alkoxides and carbocations .-Alcohol dehydratation .- Transformation in haloalkanes and sulfonates .- Oxidation of alcohols, diols and phenols. Thiols: properties and reactivity.- Biological importance.

ETHERS, EPOXIDES AND SULFIDES .- Nomenclature and physical properties.- Cyclic ethers as solvents.- Reactions .- Epoxides: ring opening reactions.- Sulfides: structure, synthesis and applications.

AMINES AND OTHER NITROGENATED COMPOUNDS .- Structure .- Nomenclature .- Physical properties.- Acidity and basicity of amines .- Aromatic amines.- Arenodiazonium salts as intermediates in organic synthesis.

4. Compounds with carbon-heteroatom multiple bonds

Part IV: 10h.

ALDEHYDES AND KETONES. THE CARBONYL GROUP. Nomenclature of aldehydes and ketones.- Structure of the carbonyl group.- Nucleophilic addition to the carbonyl group.- Addition of water and alcohols: acetals and hemiacetals, cyclic sugars.- Addition of carbon nucleophiles .- Addition of amines and related compounds .- Reduction and oxidation. Enols and enolates.

CARBOXYLIC ACIDS AND THEIR DERIVATIVES.- Nomenclature .- Structure .-Physical Properties .- Acidity and basicity of carboxylic acids and carboxylic acid derivatives .- Reactivity of the carboxylic group: the addition-elimination mechanism.- Transformations between carboxylic acid derivatives: acyl halides, anhydrides, esters and amides .- Reactions of carboxylic acid derivatives.

NITRILES AND ISOCYANATES. General structure and reactivity. .- CARBAMATES.- Aminoacids,peptides and proteins.-

SIMPLE AROMATIC HETEROCYCLES: Pyridine and pyrrole. Fused heteroaromatic rings: Indole,quinoline and isoquinoline.- Heterocycles with two or more heteroatoms.

5. Design and synthesis of simple organic compounds

Part V:

INTRODUCTION TO ORGANIC SYNTHESIS. Planning a synthesis. The disconnection approach. Synthesis strategies. Species with electrophilic and species with nucleophilic carbon.

CHEMOSELECTIVITY AND PROTECTING GROUPS. Protecting groups of alcohols and amines.- Carbonyl protecting groups. Examples.

6. Laboratory sessions

Part VI: 20h
- Safety in the organic chemistry laboratory.
- Introduction to the experimental techniques for the separation and purification and identification of organic compounds
- Experiments in organic synthesis
- Identification of the obtained products

7. PRACTICAL SESSIONS OF SEMINARS

Block VII: 8h
STRUCTURAL ANALYSIS OF ORGANIC COMPOUNDS. Application of the techniques of mass spectrometry, UV-visible, IR and NMR to the determination of the structures of simple organic compounds.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	56,00	100
Seminars	36,00	100
Laboratory practices	20,00	100
Tutorials	6,00	100
Development of group work	14,00	0
Study and independent work	8,00	0
Preparation of evaluation activities	40,00	0
Preparing lectures	44,00	0
Preparation of practical classes and problem	70,00	0
TOTAL	**294,00**	

TEACHING METHODOLOGY

Lectures .-The professor will introduce the topics under study,particularly those aspects of particular complexity,using the most suitable tools of information and communication. The professor will indicate the points for the students to review prior to attending each class. Student participation will be encouraged.

Practice problems: These classes will address the application of the topics introduced in the lectures. The students should have worked the problems out in advance. The professor will guide the problem solving work, which should preferably be discussed by the students, either in groups or individually. These classes require substantial student's personal work. 28 hours.

Tutorials.- Students will attend in small groups. The professor will solve the doubts and guide students on the most useful methods for studying the different topics and solving the problems. The teacher may raise issues, specific exercises or written jobs to beworked out by the students.The teacher will evaluate the process of learning in a global way.

Seminars .- Seminars can be used for the introduction to the spectroscopic techniques and their application to the structural determination. Complementary activities (management of drawing programs and computer modeling, molecular models, discussion of current issues etc.) may also be carried out as well. 8 hours.

Laboratory .-Introduction to the organic chemistry laboratory. The student will learn the basic experimental techniques for the preparation, isolation and purification of simple organic compounds, and also the risks associated with handling and use of these products and techniques.

EVALUATION

The assessment of student learning will take into account all the aspects outlined in the methodology described above.

- 10% of the grade will come from direct evaluation of teacher in classes and tutorials. In this evaluation different aspects shall be taken into account:

* participation in the discussions raised in classes;

* progress in the use of the organic chemistry language;

* ability to solve problems and ask questions;

- 10% of the grade will be obtained from the participation and the work developed in the seminars;

- 15% of the note corresponds to the attendance and participation in practical classes at the laboratory. A minimum of 40% of the maximum score is required for pass the practice exam. Attendance to these activities is required to pass the course, unless the student had already attended and passed them. Students that have already succeded practical sesión in the previous three courses are not forced to do it again. The obtained mark (from practical part) will remain for three years.

The evaluation of the laboratory work will consider:

*Experimental skills, participation and observation of the safety rules (40%).

*Preparation in advance of the laboratory work, and laboratory notebook (20%).

*Exam on the experimental techniques (40%).

- 65% of the grade will be obtained from the examinations results. The exams will be coordinated by the professors of the different groups, although they will not be necessarily identical.

Exams: two exams in the first semester and one in the second semester (the first final exam). In order to pass the course the student must obtain a score equal to or greater than 4/10 in each exam. In any situation the global score must be higher than 4.5/10 .The final note will sum up the exam scores plus the marks corresponding to practical classes, seminars and direct evaluation.

The scores obtained in the partial exams will be maintained for the second final exam, to be held on dates set by the center(probably July 2014). The notes of direct evaluation will be maintained in this case. In the case that the student had performed the scheduled activities (practical classes, seminars) but failed to attend the final exam, he/she will be considered “No presentado” in the first round and “Suspenso” in the second one.

REFERENCES

Basic

- K. P. C. Vollhardt, N.E. Schore. Química Orgánica (5ª ed.). Ed. Omega (2007).
- F.A. Carey. Química Orgánica (6ª ed.) Mc Graw-Hill (2006).
- L. G. Wade Jr. Química Orgánica(5ª ed.). Ed. Pearson Prentice Hall (2004)
  P.Yurkanis Bruice Química Orgánica (5ª ed.). Ed. Pearson Prentice Hall (2008)
  D. Klein Química Orgánica (1ª ed.) Ed. Panamericana (2012).

Additional

- ChemBioOffice Ultra, PerkinElmer (CambridgeSoft) Amplia selección de aplicaciones y funcionalidades que permite estudiar, dibujar, formular, modelar y editar estructuras moleculares químicas y biológicas."
- J.R. Pedro y G. Blay 200 Problemas de Determinación estructural de Compuestos Orgánicos. Ed Visión Libro 2010 (Madrid)
- W.R.Peterson. Formulación y nomenclatura química orgánica. (4ª ed) Ed. Reverte (2016)